Topics in Deployable ML: Min-Max Optimization I (Lecture 8)

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Motivation for this Lecture

Minimization is to current Al what <u>min-max optimization</u> is to future Al

- Minimization: Al agent is learning in a stationary environment
- Min-max optimization: Al agent is learning in a *changing* environment
- Why changing?
 - Because noise/adversaries poison or corrupt the data [*c.f. lecture 4*]
 - Because the agent is optimizing against another agent with conflicting interests
 - Because the agent wants to enforce constraints on the learning outcome, e.g. GANs, private release of data etc.

Generative Adversarial Networks

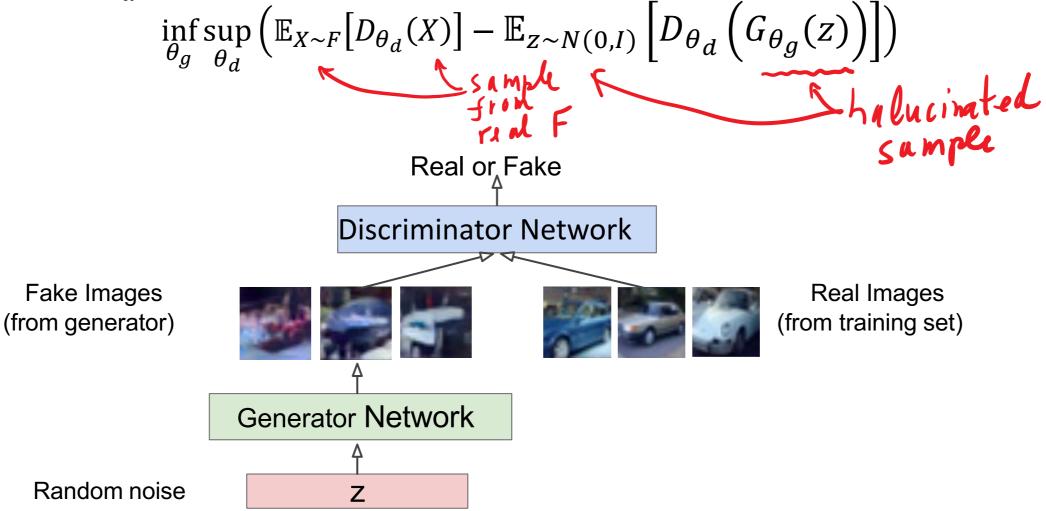
 Algorithms mapping white noise to random high-dimensional objects with structure:

$$z \sim N(0, I_{100 \times 100}) \longrightarrow$$
 face GAN \longrightarrow is a face of the second second

- If you want, what human imagination does (presumably)
- Trained using samples (e.g. faces) from true high-dimensional distribution with structure (e.g. natural face images)

 $z \sim N(0, I)$ E.g. Wasserstein GAN face GAN [Arjovsky-Chintala-Bottou'17]

• A *game* between a *Generator* deep NN, w/ parameters θ_g , and a *Discriminator* deep NN, w/ parameters θ_d :



- **Training**: generator and discriminator run gradient descent and ascent respectively to update their parameters θ_g , θ_d ; expectations are approximated by finite sample averages
- even ignoring expectation approximation errors, will paired gradient descent/ascent dynamics converge? to what?

- Motivation
- Min-Max Theorem
- No-Regret Learning and Online Convex Optimization
- Back to Min-Max Optimization

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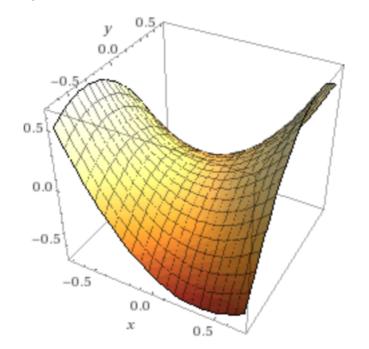
The Min-Max Theorem

• **[von Neumann 1928]:** If $X \subset \mathbb{R}^n$, $Y \subset \mathbb{R}^m$ are compact and convex, and $f: X \times Y \to \mathbb{R}$ is convex-concave (i.e. f(x, y) is convex in x for all y and is concave in y for all x), then

$$\min_{x \in X} \max_{y \in Y} f(x, y) = \max_{y \in Y} \min_{x \in X} f(x, y)$$

• Min-max optimal point (x, y) is essentially unique (unique if f is strictly convex-concave, o.w. a convex set of solutions); value always unique

• E.g.
$$f(x, y) = x^2 - y^2 + x \cdot y$$

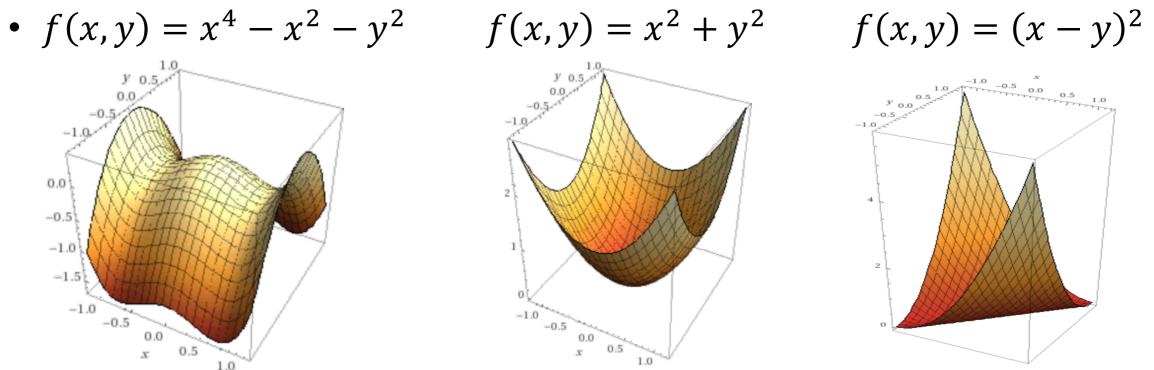


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- If f is not convex concave all bets are off



The Min-Max Theorem

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- Min-max optimal point (x, y) is essentially unique (unique if f is strictly convex-concave, o.w. a convex set of solutions); value always unique
- Min-max points = equilibria of zero-sum game where min player pays max player f(x, y)
- von Neumann: "As far as I can see, there could be no theory of games ... without that theorem ... I thought there was nothing worth publishing until the Minimax Theorem was proved"
- When f is bilinear, i.e. $f(x, y) = x^T A y + b^T x + c^T y$ and X, Y polytopes
 - **[von Neumann-Dantzig 1947, Adler IJGT'13]:** Minmax ⇔ strong LP duality
 - min-max solutions can be found w/ Linear Programming and vice versa
 - mathematical structure arguably crucial in recent success of computers beating humans in two-player zero-sum games (chess, poker, go)

The Min-Max Theorem (distributed dynamics or very high dimensions)

 [Brown RAND'49]: proposes *fictitious play* as a method to solve bilinear case on product of simplices:

$$\min_{x \in \Delta_n} \max_{y \in \Delta_m} x^T A y = \max_{y \in \Delta_m} \min_{x \in \Delta_n} x^T A y$$

- Fictitious play: $(x_t, y_t)_{t=1,...}$ where for all t:
 - $x_t \in \operatorname{argmin} \sum_{\tau < t} f(\cdot, y_{\tau})$
 - $y_t \in \operatorname{argmax} \sum_{\tau < t} f(x_{\tau}, \cdot)$
- [Robinson Annals of Math'51]: shows fictitious play converges in bilinear case in an average sense: $\frac{1}{t} \sum_{\tau} f(x_{\tau}, y_{\tau}) \rightarrow \min \max f(x, y)$
- [Karlin'59]: conjectures convergence rate is $\sim 1/\sqrt{t}$
- **[Daskalakis-Pan FOCS'14]:** actually exponentially slow $(\sim 1/t^{1/m+n})$
- Faster methods?

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Online Convex Optimization

- Game between learner and nature [min player's perspective in min max f(x, y)]
- Every day $t = 1, \dots, T$:
 - Learner chooses $x_t \in X \subset \mathbb{R}^n$
 - World chooses convex function $f_t(\cdot)$ [in min-max problem $f_t(\cdot) \equiv f(\cdot, y_t)$]
 - Learner incurs loss $f_t(x_t)$; observes $f_t(\cdot)$
- Learner's goal:
 - $\frac{1}{T} \sum_{t} f_t(x_t) \approx \frac{1}{T} \sum_{t} \min f_t(\cdot)$ Unattainable (see notes)

• $\frac{1}{\tau} \sum_t f_t(x_t) \approx \frac{1}{\tau} \min \sum_t f_t(\cdot)$

attainable [and sufficient for min-max]

• $\frac{1}{\tau}\sum_t f_t(x_t) - \frac{1}{\tau}\min\sum_t f_t(\cdot)$:

average regret of the learner

• **Theorem:** Suppose, $\forall t = 1, ..., T$, f_t is convex and L-Lipschitz. There exists learning algorithm such that $\frac{1}{T}\sum_t f_t(x_t) - \min \frac{1}{T}\sum_t f_t(\cdot) \le O_X\left(\frac{L}{\sqrt{T}}\right)$ **No-regret property** (means avg regret $\rightarrow 0$)

How to achieve no regret?

Setting: Every day t = 1, ..., T:

- learner chooses $x_t \in X$
- world chooses L-Lipschitz convex f'n $f_t(\cdot)$
- learner loses $f_t(x_t)$; observes $f_t(\cdot)$

Goal: $\frac{1}{T}\sum_{t} f_t(x_t) - \frac{1}{T}\min\sum_{t} f_t(\cdot) \to 0$

- Idea 1: follow-the-leader (FTL): on day t choose $x_t \in \arg \min \sum_{\tau < t} f_{\tau}(\cdot)$
 - Average regret doesn't go to 0 ⁽³⁾ [see notes]
 - Issue: overfitting
 - learner's actions move around abruptly
- Idea 2: regularize!
- follow-the-regularized-leader (FTRL): on day t choose

$$x_t \in \arg\min\left[\sum_{\tau < t} f_{\tau}(\cdot) + \frac{1}{\eta} \cdot R(\cdot)\right]$$

for some η and strongly convex regularization function $R(\cdot)$

Follow-the-Regularized Leader (FTRL)

Setting: Every day t = 1, ..., T:

- learner chooses $x_t \in X$
- world chooses L-Lipschitz convex f'n $f_t(\cdot)$
- learner loses $f_t(x_t)$; observes $f_t(\cdot)$

Goal:

 $\frac{1}{\tau}\sum_t f_t(x_t) - \frac{1}{\tau}\min\sum_t f_t(\cdot) \to 0$

- **Def:** $R: X \to \mathbb{R}$ is α -strongly convex w.r.t. norm $\|\cdot\|$ iff for all $x, x_0 \in X$: $R(x) \ge R(x_0) + \nabla R(x_0)^T \cdot (x - x_0) + \frac{\alpha}{2} \|x - x_0\|^2$ $e.g.1: R(x) = x^2/2$ e.g.2: R(x) = -H(x),
- **FTRL:** On day *t* choose: $x_t \in \arg \min \left[\sum_{\tau < t} f_{\tau}(\cdot) + \frac{1}{\eta} \cdot R(\cdot) \right]$, for some parameter η , and some strongly convex regularization function $R(\cdot)$
- **Theorem:** Suppose, $\forall t = 1, ..., T$, f_t is convex and L-Lipschitz w.r.t. some norm $\|\cdot\|$, and R is 1-strongly convex w.r.t. $\|\cdot\|$. Then FTRL with parameter η satisfies:

$$\sum_{t} f_t(x_t) - \min \sum_{t} f_t(\cdot) \le \frac{\max_X R(\cdot) - \min_X R(\cdot)}{\eta} + \eta \cdot L^2 \cdot T$$

• set $\eta = L^{-1} \cdot \sqrt{(\max R(\cdot) - \min R(\cdot))/T}$ to balance terms on RHS, and get average regret of $L \cdot \sqrt{(\max R(\cdot) - \min R(\cdot))/T}$

Follow-the-Regularized Leader (FTRL)

Setting: Every day t = 1, ..., T:

- learner chooses $x_t \in X$
- world chooses L-Lipschitz convex f'n $f_t(\cdot)$
- learner loses $f_t(x_t)$; observes $f_t(\cdot)$

Goal:

 $\frac{1}{\tau}\sum_t f_t(x_t) - \frac{1}{\tau}\min\sum_t f_t(\cdot) \to 0$

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- FTRL special cases:
 - FTRL w/ ℓ_2^2 -regularizer \approx online gradient descent [notes]
 - FTRL on simplex w/ negative entropy regularizer = multiplicative-weightsupdate method

FTRL and Min-Max

- Suppose f(x, y) convex-concave, and both x and y players run FTRL
- Namely:
 - the x-player chooses x_t by applying FTRL to observed losses $f(\cdot, y_t)$
 - the y-player chooses y_t by applying FTRL to observed losses $-f(x_t, \cdot)$
- **Theorem:** If x and y player play as above, then:
 - $\frac{1}{T} \sum_{t=1}^{T} f(x_t, y_t) = \min_{x} \max_{y} f(x, y) \pm O(\frac{1}{\sqrt{T}})$
 - Moreover, the average strategies $\bar{x}_T = \frac{1}{T} \sum_t x_t$ and $\bar{y}_T = \frac{1}{T} \sum_t y_t$ are a $O(\frac{1}{\sqrt{T}})$ -approximate Nash equilibrium, i.e.
 - $f(\bar{x}_T, \bar{y}_T) \le \min f(\cdot, \bar{y}_T) + O(\frac{1}{\sqrt{T}})$
 - $f(\bar{x}_T, \bar{y}_T) \ge \max f(\bar{x}_T, \cdot) O(\frac{1}{\sqrt{T}})$
- Proof: notes

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Challenges in GAN Training

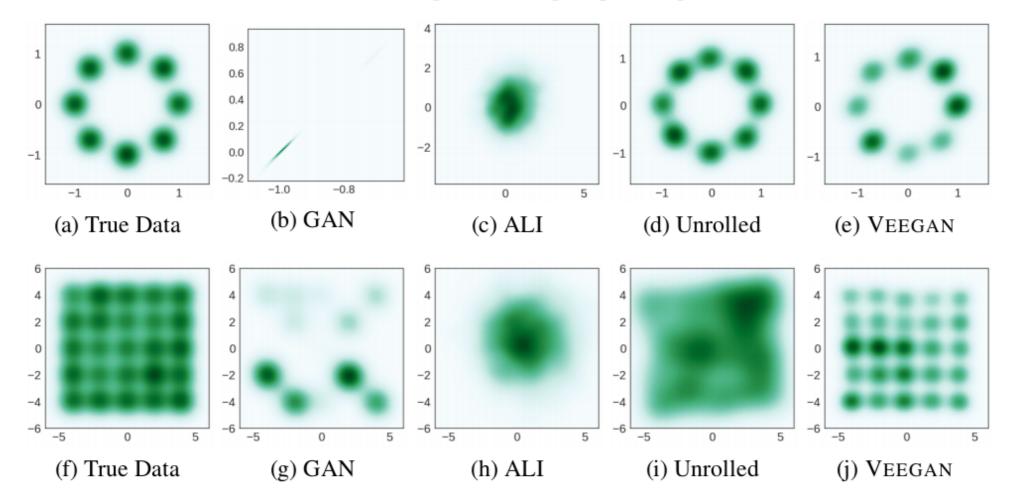
• Recall, they are defined by setting up a *game* between a *Generator* deep NN, w/ parameters θ_g , and a *Discriminator* deep NN, w/ parameters θ_d :

$$\inf_{\theta_g} \sup_{\theta_d} (f(\theta_g, \theta_d))$$

- **Training**: generator and discriminator run online gradient descent and ascent respectively and in parallel to update their parameters θ_g , θ_d
- **Question:** will paired online gradient descent/ascent style dynamics converge? to what?
- Challenge 1: objective function $f(\theta_g, \theta_d)$ isn't convex-concave
 - So what is the goal?
 - 1. [Daskalakis-Panageas NeurIPS'18] study local saddles (don't necessarily exist)
 - 2. [Jin-Netrapali-Jordan'19] study local min of $\max_{y} f(\cdot, y)$ function (exist under mild conditions)
 - E.g. $\min_{x \in [0,1]} \max_{y \in [0,1]} -(x y)^2$: 1 doesn't exist, 2 does exist
 - Are above reasonable? Well,...
 - under 1: maybe my trained discriminator cannot locally improve discrimination, but some other discriminator (e.g. your brain) can discriminate really well between real and generated images (locally optimal discrimination isn't sufficient)
 - under 1 and 2: if my trained discriminator is optimal and my trained generator is locally optimal, it might just have given up

Mode Collapse

Figure 2: Density plots of the true data and generator distributions from different GAN methods trained on mixtures of Gaussians arranged in a ring (top) or a grid (bottom).



VEEGAN: Reducing Mode Collapse in GANs using Implicit Variational Learning Akash Srivastava, Lazar Valkov, Chris Russell, Michael U. Gutmann, Charles Sutton

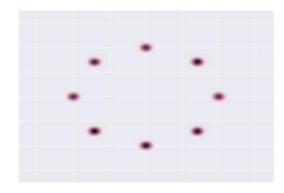
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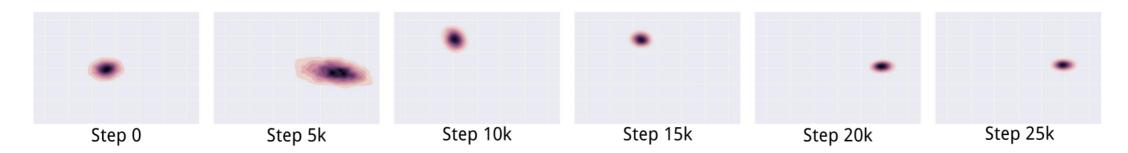
$$\inf_{\theta_g} \sup_{\theta_d} (f(\theta_g, \theta_d))$$

- Training: generator and discriminator run gradient descent and ascent respectively to update their parameters θ_g , θ_d
- Question: even ignoring expectation approximation errors, will paired gradient descent/ascent style dynamics converge? to what?
- Challenge 2: oscillations
 - even if $f(\theta_g, \theta_d)$ is convex-concave, we only argued that gradient/descent ascent, or FTRL converge in an **average sense**
 - i.e. $\overline{\theta_g}_T = \frac{1}{T} \sum_t \theta_{g_t}$ and $\overline{\theta_d}_T = \frac{1}{T} \sum_t \theta_{d_t}$ would be an approximate saddle but we didn't provide any guarantees for the last iterate $(\theta_{g_T}, \theta_{d_T})$...
 - and there aren't such guarantees generically

Training Oscillations: Gaussian Mixture



True Distribution: Mixture of 8 Gaussians on a circle



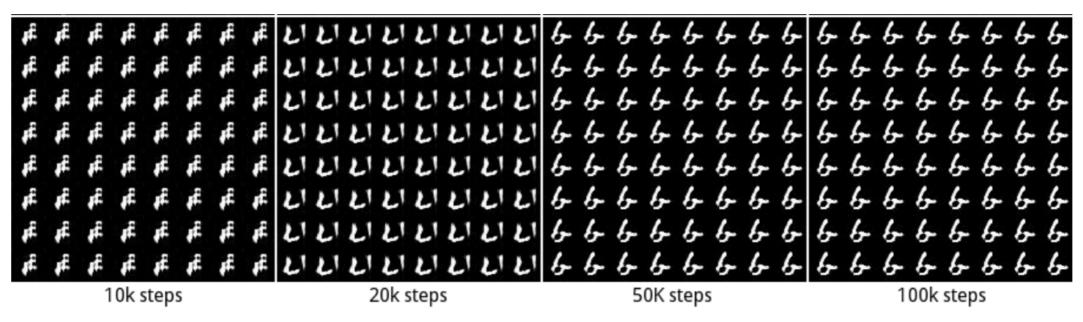
Output Distribution of standard GAN, trained via gradient descent/ascent dynamics: *cycling through modes at different steps of training*

from [Metz et al ICLR'17]

Training Oscillations: Handwritten Digits



True Distribution: MNIST

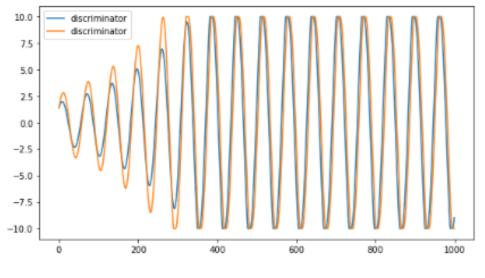


Output Distribution of standard GAN, trained via gradient descent/ascent dynamics cycling through "proto-digits" at different steps of training

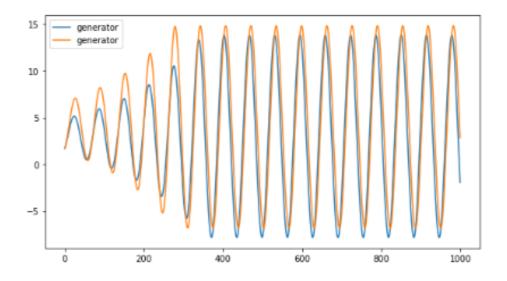
from [Metz et al ICLR'17]

Training Oscillations: even for bilinear objectives!

- **True distribution:** isotropic Normal distribution, namely $X \sim \mathcal{N}\left(\begin{bmatrix} 3 \\ 4 \end{bmatrix}, I_{2 \times 2} \right)$
- Generator architecture: $G_{\theta}(Z) = \theta + Z$ (adds input Z to internal params)
- **Discriminator architecture**: $D_w(\cdot) = \langle w, \cdot \rangle$ (inear projection)
- W-GAN objective: $\min_{\theta} \max_{w} \mathbb{E}_{X}[D_{w}(X)] \mathbb{E}_{Z}[D_{w}(G_{\theta}(Z))]$ = $\min_{\theta} \max_{w} w^{T} \cdot \left(\begin{bmatrix} 3 \\ 4 \end{bmatrix} - \theta \right)$ convex-concave function

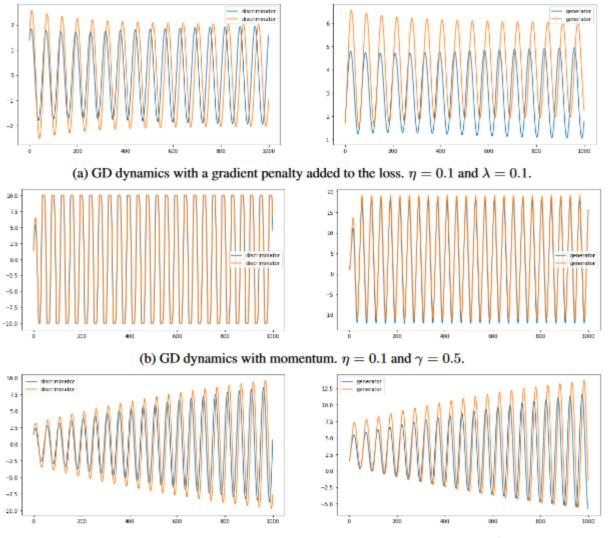


Gradient Descent Dynamics

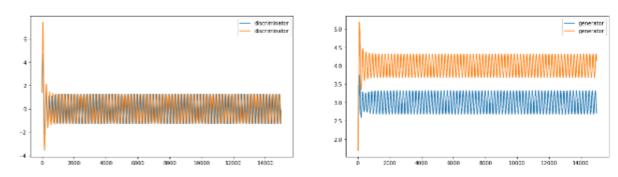


from [Daskalakis, Ilyas, Syrgkanis, Zeng ICLR'18]

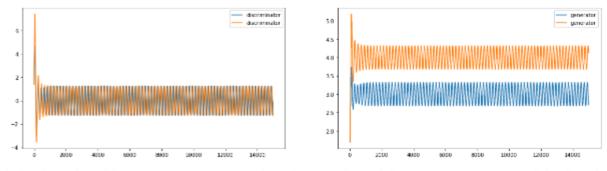
Training Oscillations: persistence under many variants of Gradient Descent

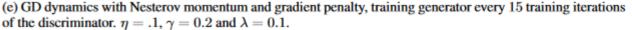


(c) GD dynamics with momentum and gradient penalty. $\eta = .1$, $\gamma = 0.2$ and $\lambda = 0.1$.



(d) GD dynamics with momentum and gradient penalty, training generator every 15 training iterations of the discriminator. $\eta = .1$, $\gamma = 0.2$ and $\lambda = 0.1$.





from [Daskalakis, Ilyas, Syrgkanis, Zeng ICLR'18]

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- Min-Max Theorem
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 - Last Iterate Convergence

Gradient Descent w/ Negative Momentum

• Variant of gradient descent:

$$\forall t: x_{t+1} = x_t - \eta \cdot \nabla f(x_t) + \eta/2 \cdot \nabla f(x_{t-1})$$

- Interpretation: undo today, some of yesterday's gradient; ie negative momentum
- Gradient Descent w/ negative momentum
 - = Optimistic FTRL w/ ℓ_2^2 -regularization [Rakhlin-Sridharan COLT'13,

Syrgkanis et al. NeurIPS'15]

= unconstrained Popov's method [Popov 1980]

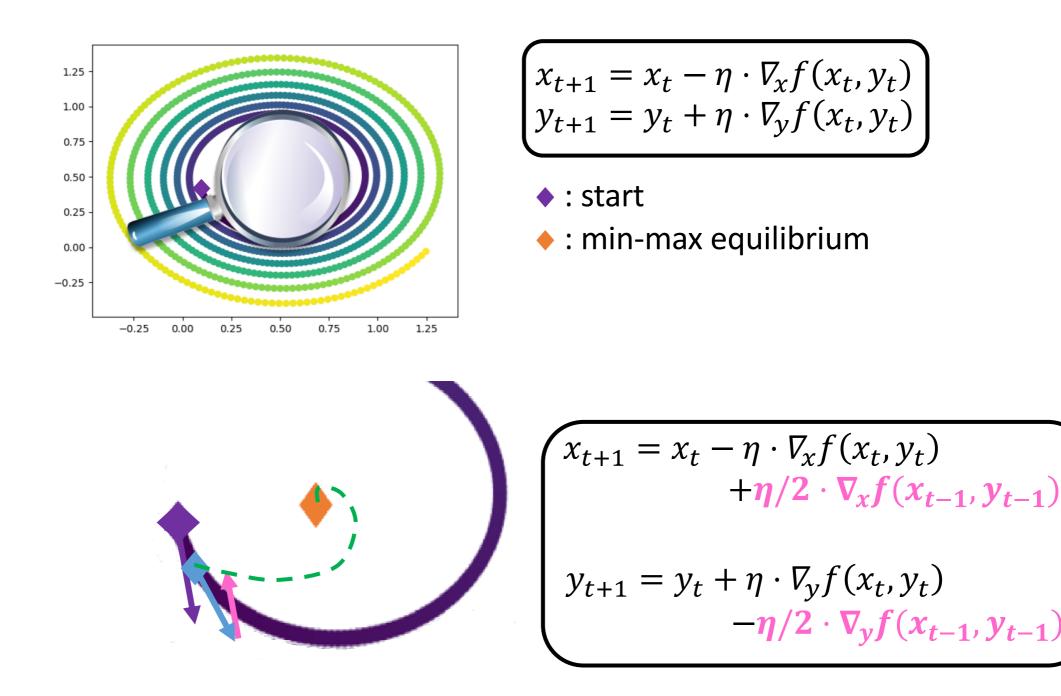
≈ extra-gradient method [Korpelevich'76, Chiang et al COLT'12, Mertikopoulos et al'18]

= mirror prox method w/ ℓ_2^2 -regularization [Nemirovski'04, Mohtari-Ozdaglar-Pattathil'19]

• Does it help in min-max optimization?

Negative Momentum: why it could help

• E.g. $f(x, y) = (x - 0.5) \cdot (y - 0.5)$

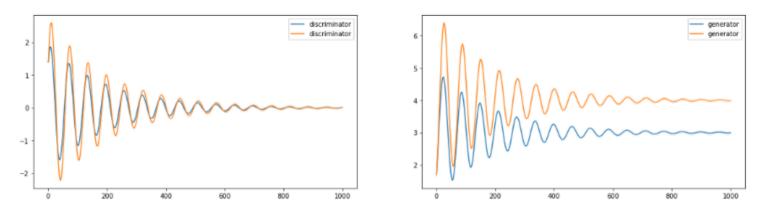


Negative Momentum: convergence

• Optimistic gradient descent-ascent (OGDA) dynamics:

$$\forall t: \ x_{t+1} = x_t - \eta \cdot \nabla_x f(x_t, y_t) + \frac{\eta}{2} \cdot \nabla_x f(x_{t-1}, y_{t-1}) \\ y_{t+1} = y_t + \eta \cdot \nabla_y f(x_t, y_t) - \frac{\eta}{2} \cdot \nabla_y f(x_{t-1}, y_{t-1})$$

- **[Daskalakis-Ilyas-Syrgkanis-Zeng ICLR'18]: OGDA** exhibits last iterate convergence & fast rates for *unconstrained* bilinear games: $\min_{x \in \mathbb{R}^n} \max_{y \in \mathbb{R}^m} f(x, y) = x^T A y + b^T x + c^T y$
- [Liang-Stokes AISTATS'19, Gidel et al AISTATS'19]: ...convergence rate is geometric if A is well-conditioned, extends to strongly convex-concave functions f(x, y)
- E.g. in previous isotropic Gaussian case: $X \sim \mathcal{N}((3,4), I_{2\times 2}), G_{\theta}(Z) = \theta + Z,$ $D_w(\cdot) = \langle w, \cdot \rangle$



Negative Momentum: convergence

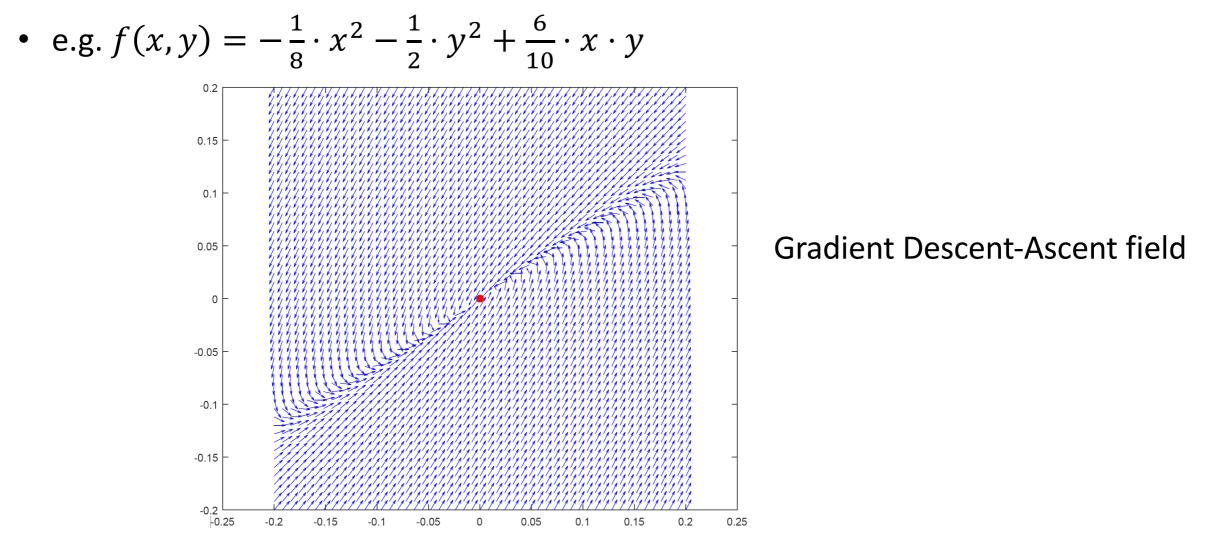
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- **[Daskalakis-Ilyas-Syrgkanis-Zeng ICLR'18]: OGDA** exhibits last iterate convergence & fast rates for *unconstrained* bilinear games: $\min_{x \in \mathbb{R}^n} \max_{y \in \mathbb{R}^m} f(x, y) = x^T A y + b^T x + c^T y$
- [Liang-Stokes AISTATS'19, Gidel et al AISTATS'19]: ...convergence rate is geometric if A is well-conditioned, extends to strongly convex-concave functions f(x, y)
- [Mohtari et al'19]: ...ditto for extra-gradient, mirror-prox methods
- **[Daskalakis-Panageas ITCS'19]:** *Projected* OGDA exhibits last iterate convergence even for *constrained* bilinear games: $\min_{x \in \Delta_n} \max_{y \in \Delta_m} x^T A y = \text{all linear programming}$
- **General Comment:** asymptotic convergence results were known already by Korpelevich and Popov for extragradient and negative momentum respectively
- [w/ Jelena Diakonikolas, Mike Jordan]: results for general constraints + convergence rates + general Bregman divergences

Negative Momentum: in the Wild

- Can try optimism for non convex-concave min-max objectives f(x, y)
- Issue [Daskalakis, Panageas NeurIPS'18]: No hope that stable points of OGDA or GDA are only local min-max points



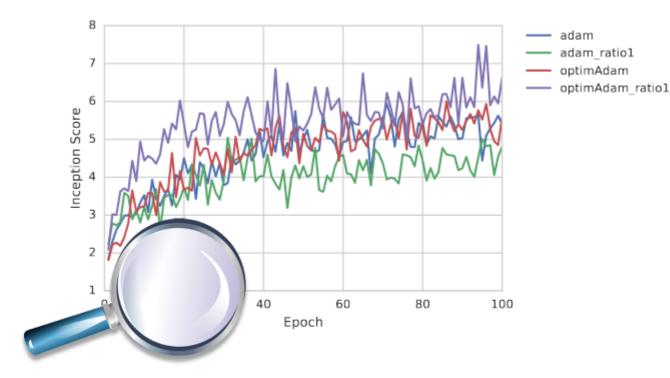
- Nested-ness: Local Min-Max ⊆ Stable Points of GDA ⊆ Stable Points of OGDA
- (stability refers to linear stability and left inclusion for strong local min-max points)

Negative Momentum: in the Wild

- Can try optimism for non convex-concave min-max objectives f(x, y)
- Issue [Daskalakis, Panageas NeurIPS'18]: No hope that stable points of OGDA or GDA are only local min-max points
 - Local Min-Max \subseteq Stable Points of GDA \subseteq Stable Points of OGDA
- also [Adolphs et al. 18]: left inclusion
- **Question:** identify first-order method converging to local min-max w/ probability 1
- While this is pending, evaluate optimism in practice...
- [Daskalakis-Ilyas-Syrgkanis-Zeng ICLR'18]: propose optimistic Adam
 - Adam, a variant of gradient descent proposed by [Kingma-Ba ICLR'15], has found wide adoption in deep learning, although it doesn't always converge [Reddi-Kale-Kumar ICLR'18]
 - Optimistic Adam is the right adaptation of Adam to "undo some of the past gradients"

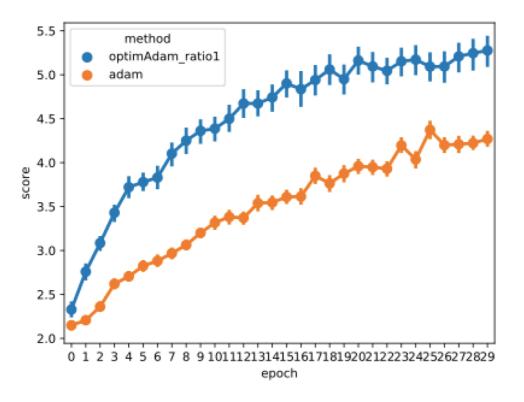
Optimistic Adam on CIFAR10

- Compare Adam, Optimistic Adam, trained on CIFAR10, in terms of Inception Score
- No fine-tuning for Optimistic Adam, used same hyper-parameters for both algorithms as suggested in Gulrajani et al. (2017)



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(b) Sample of images from Generator of Epoch 94, which had the highest inception score.

Figure 14: The inception scores across epochs for GANs trained with Optimistic Adam (ratio 1) and Adam (ratio 5) on CIFAR10 (the two top-performing optimizers found in Section 6) with 10%-90% confidence intervals. The GANs were trained for 30 epochs and results gathered across 35 runs.

 Further supporting evidence for negative momentum methods by [Gidel et al. AISTATS'19]